

MATERIAL INNOVATION USING GENERATIVE MATERIAL DESIGN - A DIGITAL TWIN

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Abstract: Despite its potential to transform society, materials research suffers from a major drawback: its long research timeline. Recently, machine-learning techniques have emerged as a viable solution to this drawback. As we know that the digital twin is a digital model of an intended or actual real-world physical product, system, or process (a physical twin) that serves as the effectively indistinguishable digital counterpart of it for practical purposes, such as simulation, integration, testing, monitoring, and maintenance. Using that concept we have adopted a Generative Material Design - a cloud-based integrated solution that optimizes materials design and discovery combining the virtual and real world — potentially saving millions of research dollars. This process includes: a) Combine advanced data science, machine learning, cheminformatics and structure-based modeling to explore chemical space, b) Automate the virtual creation, testing and selection of novel small molecules, c) Reduce the cost of physical testing and then revalidate with laboratory including formulation/reformulation. *This talk will show real life examples of utilization of this digital twin for designing materials.*